Quantum phase diffusion of a Bose system: beyond the Hartree-Fock-Bogoliubov approximation

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Abstract

A diffusion process is usually assumed for the phase of the order parameter of a Bose system of finite size. The theoretical basis is limited to the so called Bogoliubov approximation. We show that a suitable generalization of the Hartree-Fock-Bogoliubov approach recovers phase diffusion.

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I. INTRODUCTION

Bose-Einstein condensation (BEC) of weakly interacting atom systems attracted a large attention since the studies on liquid Helium, and a renewed interest stimulated by experimental observations of condensation of trapped alkali atoms [1, 2, 3].

Relevant theoretical approaches have been reviewed by Griffin [4]. The condensate is usually considered in a coherent state whose amplitude satisfies a nonlinear Schrodinger equation [5, 6, 7]. Quantum fluctuations determine the instability of this state, known as phase diffusion (PD), as analyzed in the work of Lewenstein and You [8]. This instability is expected in systems in restricted geometries, where a real symmetry-breaking phase cannot occur. In Ref. [8], a gapless approximation, the Bogoliubov or the Hartree-Bogoliubov (HB), has been shown to exhibit PD, and it is also noted that a complete self-consistent approximation, the Hartree-Fock-Bogoliubov (HFB), has a gapped which spectrum prevents PD. However, it must be rejected because does not satisfy the number conservation law [4].

In a different contest [9], we recently described the possibility of observing BEC and quasisuperfluid behavior in two-mode photon systems. In that case the single mode approximation can be made. Thus, we obtain the zero-dimensional version of the problem of two interacting Bose condensates [10, 11, 12]. This model can be also viewed as a particular case of systems of itinerant polaritons [13, 14]. We showed that in the study of the evolution of an initial coherent state, there is, in the condensate phase, an initial time range where the effect of a symmetry-breaking field can be neglected, and PD should be observed.

On the other hand, the Bogoliubov transformation amounts to a rotation in the particle degrees of freedom which leads to quasi-particles. It is easily shown that the rotation angle becomes infinite in the limit of vanishing symmetry-breaking field in the HB approximation, while it is kept finite in the HFB approximation [15, 16]. Thus, quantities related to the condensate fluctuations, as for instance $\langle aa \rangle$ and $\langle a^{\dagger}a^{\dagger} \rangle$, in HB are actually diverging in the limit of vanishing symmetry-breaking field. As a consequence, the instability of the condensate is strongly enhanced with respect to PD. In spite of the weakness of the theoretical background, the existence of PD is widely accepted and used to explain several experimental and theoretical results [17, 18, 19].

The aim of this work is to show that a self-consistent approximation can be introduced which satisfies both the requirements of finite rotation and the absence of a gap in the excitation spectrum. This latter feature is a direct consequence of the validity of the continuity equation. This result can be achieved within a truncation procedure of the equations of motion which considers linear and bilinear quantities in the creation and annihilation operators space. Higher order terms are taken into account by means of the factorization in the original picture of creation and annihilation particles operators, or alternatively, by normal ordering of corresponding quantities in the quasi-particle operators.

The structure of the paper is the following. In Sec. II we introduce the general model and discuss the problem of PD in the Bogoliubov and HFB approximations. In Sec. III we first establish the equations of motion truncation, and then we show how PD is mainteined in the extended selfconsitent theory. Then, we conclude the paper in Sec. IV.

II. THE MODEL

We first introduce the problem in the context of interacting photon systems [9]. Two e.m. modes interacts via a tunneling term in a nonlinear medium:

$$H = \omega_0 \left(a_1^{\dagger} a_1 + a_2^{\dagger} a_2 \right) - w \left(a_1^{\dagger} a_2 + a_2^{\dagger} a_1 \right) + g \left(a_1^{\dagger} a_1 + a_2^{\dagger} a_2 \right)^2 \tag{1}$$

Through a canonical transformation H reduces to

$$H = (\omega_0 - w) a^{\dagger} a + (\omega_0 + w) b^{\dagger} b + g \left(a^{\dagger} a + b^{\dagger} b \right)^2$$
 (2)

where $a=(a_1+a_2)/\sqrt{2}$ and $b=(a_1-a_2)/\sqrt{2}$. If the value of the hopping constant w exceeds the mode energy ω_0 , the the vacuum for the mode a is unstable. Under these conditions, by applying the Bogoliubov approximation to a coherent state for the mode a, a phase diffusion phenomenon appears [8]. The interaction between a and b can be seen as a particular case of interaction between condensate and quasi-particles in Bose particle systems in the limit where only one quasi-particle mode is considered. Taking into account that the ground state of the isolate b system is the vacuum, we concentrate ourselves on the the parts of H concerning only the mode a: $H_a=\omega_0'a^{\dagger}a+ga^{\dagger 2}a^2-\lambda\left(a+a^{\dagger}\right)$, where $\omega_0'=\omega_0-w+g$, and where we are considering explicitly a symmetry-breaking field. This field does not represent a purely mathematical tool introduced to describe the emergence of a superfluid phase, as usual in boson particles systems, but it can be physically realized through the interaction of the e.m. modes with a "classical" non-fluctuating electron current

[20]. An exact solution for the evolution of a coherent state is not known in the presence of the symmetry-breaking field, and different approximations can be made. A constraint which should be verified by any approach is represented by the continuity equation

$$\frac{da^{\dagger}a}{dt} = -i\lambda \left(a - a^{\dagger}\right) \tag{3}$$

We observe first that in the limit of vanishing nonlinearity the ground state reduces to a coherent state, that is to the vacuum of a Hamiltonian where the degrees of freedom have been translated. Then, having in mind a weak-coupling theory, we perform the translation $a \to a + \nu$. The new Hamiltonian is

 $H = E_0 + H_1 + H_2 + H_3 + H_4$, where

$$E_0 = \omega_0' \nu^2 + g \nu^4 - 2\lambda \nu, \tag{4}$$

$$H_1 = \left(a^{\dagger} + a\right) \left(\omega_0' \nu + 2g\nu^3 - \lambda\right), \tag{5}$$

$$H_2 = \omega_0' a^{\dagger} a + g \nu^2 \left(4n_{\alpha} + a^{\dagger 2} + \alpha^2 \right),$$
 (6)

$$H_3 = 2g\nu \left(a^{\dagger 2}a + a^{\dagger}a^2\right),\tag{7}$$

$$H_4 = ga^{\dagger 2}a^2. (8)$$

In this new representation the continuity equation reads as

$$\frac{da^{\dagger}a}{dt} + \nu \left(\frac{da}{dt} + \frac{da^{\dagger}}{dt}\right) = -i\lambda \left(a - a^{\dagger}\right)$$

The occurrence of BEC implies $g\nu^2$ finite even for small g.

The Bogoliubov approximation amounts to take into account terms of order $g\nu^2$ and to neglect terms of order \sqrt{g} and g. In this limit we can disregard H_3 and H_4 . The condensate amplitude ν can be fixed by minimizing E_0 :

$$\omega_0'\nu + 2g\nu^3 - \lambda = 0. (9)$$

A finite solution for the condensate amplitude ν , in the limit of vanishing λ , is obtained only for $\omega'_0 < 0$. We note that this conditions makes H_1 vanishing. Due to this choice,

$$H = \frac{\lambda}{\nu} a^{\dagger} a + g \nu^2 \left(2a^{\dagger} a + a^{\dagger 2} + a^2 \right). \tag{10}$$

For $\lambda/\nu \ll g\nu^2$ the ground state is in an eigenstate of the quadrature $x=\left(a^\dagger+a\right)/\sqrt{2}$, while the other quadrature $p=i\left(a^\dagger-a\right)/\sqrt{2}$ will have infinite fluctuations. As far as the

evolution of an initial coherent state is concerned, we obtain PD. Indeed, the coherent state of amplitude α evolves as

$$|\alpha\rangle_t = e^{i\sqrt{2}\alpha p(t)}|0\rangle = \exp\left[i\sqrt{2}\alpha\left[p(0) - 4ig\nu^2 tx(0)\right]\right]|0\rangle.$$
 (11)

The corresponding wave function in the x representation is then

$$\Psi_{\alpha}(x,t) = \frac{1}{N} \exp\left[\alpha x - \frac{x^2}{2} \left(1 - 4ig\nu^2 t\right)\right]. \tag{12}$$

On the other hand, we can characterize PD in terms of the following average quantities

$$\langle \alpha | x(t) | \alpha \rangle = x_0 \tag{13}$$

$$\langle \alpha | p(t) | \alpha \rangle = -4g\nu^2 x_0 t \tag{14}$$

$$\langle \alpha | p^2(t) | \alpha \rangle - \langle \alpha | p(t) | \alpha \rangle = \frac{1}{2} + 8g^2 \nu^4 x_0^2 t^2$$
 (15)

The HFB approximation amounts to treat H_3 and H_4 in a mean-field approximation. If one admits that higher order terms can correct H_1 and H_2 and lead to a squeezed ground state [15, 16] which can be defined as the vacuum of $\gamma = (\cosh \theta a - \sinh \theta a^{\dagger})$, H_3 becomes $2g\nu \left(2\sinh^2\theta + \cosh\theta \sinh\theta\right) \left(a + a^{\dagger}\right)$, while H_4 is now $g\left[4\sinh^2\theta a^{\dagger}a + \cosh\theta \sinh\theta \left(a^{\dagger 2} + a^2\right)\right]$. These assumptions being made, the angle θ is given by the self-consistent equation

$$\tanh 2\theta = -\frac{2g\left(\nu^2 + \sinh\theta \cosh\theta\right)}{2g\left(\nu^2 - \sinh\theta \cosh\theta\right) + \frac{\lambda}{\nu}} \tag{16}$$

which admits a finite value. While the Bogoliubov approximation satisfies the continuity equation at least in the average, this is not true for HFB, because dx/dt is proportional to $g \sinh \theta \cosh \theta$.

III. THE EXTENDED HFB SOLUTION

Now we introduce a mean field approach going beyond the simple Bogoliubov approximation without introducing a gap in the excitation spectrum. We discuss the problem starting from the equations of motion. First, we assume the existence of a finite angle θ and perform the Bogoliubov transformation. The Hamiltonian is

$$H_1 = \Lambda \left(\gamma + \gamma^{\dagger} \right) \tag{17}$$

$$H_2 = E_0 \gamma^{\dagger} \gamma + \frac{1}{2} E_1 \left(\gamma^{\dagger} \gamma^{\dagger} + \gamma \gamma \right) \tag{18}$$

$$H_3 = 2g\nu \left[\left(\gamma^3 + \gamma^{\dagger 3} \right) \frac{e^{\theta}}{2} \sinh 2\theta + \left(\gamma^{\dagger} \gamma \gamma + \gamma^{\dagger} \gamma^{\dagger} \gamma \right) e^{\theta} \left(\cosh 2\theta + \frac{\sinh 2\theta}{2} \right) \right]$$
 (19)

$$H_4 = g \left[\left(\cosh^2 2\theta + \frac{1}{2} \sinh^2 2\theta \right) \gamma^{\dagger 2} \gamma^2 + \frac{1}{4} \sinh^2 2\theta \left(\gamma^{\dagger 4} + \gamma^4 \right) + \cosh 2\theta \sinh 2\theta \left(\gamma^{\dagger} \gamma^3 + \gamma^{\dagger 3} (2) \right) \right]$$

where

$$\Lambda = \nu e^{\theta} \left[\left(\omega_0' + 2g\nu^2 \right) - \frac{\lambda}{\nu} + 2g \sinh\theta \left(e^{\theta} + \sinh\theta \right) \right], \tag{21}$$

$$E_0 = \Lambda_0 + g \left[\cosh^2 2\theta + \sinh^2 2\theta + \cosh 2\theta \left(2\sinh^2 \theta - 1 \right) \right]$$
 (22)

$$\Lambda_0 = (\omega_0' + 4g\nu^2)\cosh 2\theta + 2g\nu^2 \sinh 2\theta$$

$$E_1 = \Lambda_1 + 2g \sinh 2\theta \left(\cosh 2\theta + \sinh^2 \theta - \frac{1}{2} \right) \tag{23}$$

$$\Lambda_1 = \left(\omega_0' + 4g\nu^2\right)\sinh 2\theta + 2g\nu^2\cosh 2\theta \tag{24}$$

Then, we build a set equation of motions by limiting ourselves to consider only linear and bilinear terms and neglecting higher order operators: we choose the operators γ , γ^{\dagger} , γ^{2} , $\gamma^{\dagger 2}$, and $\gamma^{\dagger}\gamma$ as independent variables. The set of coupled equations reads

$$i\frac{d\gamma}{dt} = \Lambda + E_0\gamma + E_1\gamma^{\dagger} + 3g\nu e^{\theta}\sinh 2\theta\gamma^{\dagger 2} + g\nu e^{\theta} \left(2\cosh 2\theta + \sinh 2\theta\right) \left(\gamma^2 + 2\gamma^{\dagger}\gamma\right)$$
 (25)

$$i\frac{d\gamma^{\dagger}}{dt} = -\Lambda - E_0\gamma^{\dagger} - E_1\gamma - 3g\nu e^{\theta}\sinh 2\theta\gamma^2 - g\nu e^{\theta}\left(2\cosh 2\theta + \sinh 2\theta\right)\left(\gamma^{\dagger 2} + 2\gamma^{\dagger}\gamma\right) \tag{26}$$

$$i\frac{d\gamma^{2}}{dt} = E_{1} + 2\left[\Lambda + g\nu e^{\theta} \left(2\cosh 2\theta + \sinh 2\theta\right)\right]\gamma + 6g\nu e^{\theta} \sinh 2\theta\gamma^{\dagger}$$

$$+2\left[E_{0} + g\left(\cosh^{2} 2\theta + \frac{1}{2}\sinh^{2} 2\theta\right)\right]\gamma^{2} + 3g\sinh^{2} 2\theta\gamma^{\dagger 2}$$

$$+2\left(E_{1} + 3g\cosh 2\theta\sinh 2\theta\right)\gamma^{\dagger}\gamma \tag{27}$$

$$i\frac{d\gamma^{\dagger 2}}{dt} = -E_1 - 6g\nu e^{\theta} \sinh 2\theta \gamma - 2\left[\Lambda + g\nu e^{\theta} \left(2\cosh 2\theta + \sinh 2\theta\right)\right] \gamma^{\dagger}$$
$$-3g\sinh^2 2\theta \gamma^2 - 2\left[E_0 + g\left(\cosh^2 2\theta + \frac{1}{2}\sinh^2 2\theta\right)\right] \gamma^{\dagger 2}$$
$$-2\left(E_1 + 3g\cosh 2\theta \sinh 2\theta\right) \gamma^{\dagger} \gamma \tag{28}$$

$$i\frac{d\gamma^{\dagger}\gamma}{dt} = \Lambda \left(\gamma^{\dagger} - \gamma\right) + E_1 \left(\gamma^{\dagger 2} - \gamma^2\right) \tag{29}$$

Note that the truncation is performed after normal ordering of higher order terms. Then, the equations for the bilinear operators are not equivalent to those of the linear ones, i.e., for example, γ^2 is not simply the square of γ .

The natural choice for the parameters ν and θ cancels all the constants appearing in the above equations which should give rise to instability also for $\lambda \neq 0$. This choice corresponds to the constraints $\Lambda = 0$ and $E_1 = 0$. Due to these conditions

$$E_0 = \left(\frac{\lambda}{\nu} - 2g\sinh 2\theta\right)e^{-2\theta}.$$
 (30)

An important consequence of these constraints is the conservation of the quasi-particles number $n_{\gamma} = \gamma^{\dagger} \gamma$:

$$\frac{dn_{\gamma}}{dt} = 0\tag{31}$$

Furthermore, the value of θ is exactly that of Eq. (16).

The important feature of the previous approximation is that the continuity equation is valid independently on the satisfaction of $\Lambda = 0$ and $E_1 = 0$. Once the constraints are taken into account, the continuity equation implies

$$i\frac{\sinh 2\theta}{2}\frac{d}{dt}\left(\gamma^2 + \gamma^{\dagger 2}\right) + i\nu e^{\theta}\frac{d}{dt}\left(\gamma + \gamma^{\dagger}\right) = \lambda e^{-\theta}\left(\gamma - \gamma^{\dagger}\right). \tag{32}$$

The proof requires some tedious algebra which will be reported in appendix. It is worth to note that for $\lambda = 0$ a new constant of motion arises which is given by $(\sinh 2\theta/2) \left(\gamma^2 + \gamma^{\dagger 2}\right) + \nu e^{\theta} \left(\gamma + \gamma^{\dagger}\right)$.

In the Laplace space, the equations of motion can be summarized as follows:

$$\omega\Gamma_i(\omega) = -\sum_{k=1}^4 \phi_{ik} \Gamma_k - i\Gamma_i(t=0)$$
(33)

where $\Gamma_1 = \gamma$, $\Gamma_2 = \gamma^{\dagger}$, $\Gamma_3 = \gamma^2$, and $\Gamma_4 = \gamma^{\dagger 2}$, while the continuity equation implies

$$\frac{\sinh 2\theta}{2\nu} e^{-\theta} \left(\phi_{31} + \phi_{41}\right) + \phi_{11} + \phi_{21} = \frac{\lambda}{\nu} e^{-2\theta} \tag{34}$$

$$\frac{\sinh 2\theta}{2\nu}e^{-\theta}(\phi_{32} + \phi_{42}) + \phi_{12} + \phi_{22} = -\frac{\lambda}{\nu}e^{-2\theta}$$
(35)

$$+\phi_{13} + \phi_{23} = 0 ag{36}$$

$$\frac{\sinh 2\theta}{2\nu}e^{-\theta}(\phi_{34} + \phi_{44}) + \phi_{14} + \phi_{24} = 0 \tag{37}$$

From these equations we see that it is possible to substitute the first row of the determinant of coefficients ϕ_{ik} with the $\{(\lambda/\nu) e^{-2\theta}, -(\lambda/\nu) e^{-2\theta}, 0, 0\}$. The evolution matrix in the ω -space reads

$$D(\omega) = \left(\omega + \frac{\lambda}{\nu}e^{-2\theta}\right)D_{11}(\omega) - \frac{\lambda}{\nu}e^{-2\theta}D_{12}(\omega)$$
(38)

where D_{ik} is the minor associated to the matrix element $\omega \delta_{ik} + \phi_{ik}$. It is immediately verified the existence of a pole in the origin $(\omega = 0)$ for $\lambda \to 0$. This result is expected on the basis of general arguments (Goldstone theorem). It is worth to note that $D_{ik}(\omega)$ are finite in the present approximation.

The resiliency of PD is directly related with the presence of the pole in the origin. Indeed, by considering the evolution of p(t) we find

$$p(t) = (f_1x + f_2x^2 + f_3p^2)t + f_4p + f_5(xp + px)$$
(39)

where f_i are some nonvanishing functions of g, ν , and θ . The presence of the term proportional to t is responsible for PD. Due to this term, the variance of p on a coherent state $|\alpha\rangle$ grows as t^2 , as in the Bogoliubov case.

IV. CONCLUSIONS

In this paper we discussed the problem of phase diffusion in finite-size systems which exhibit Bose-Einstein condensation. We revised the Bogoliubov and the Hartree-Fock-Bogoliubov approximations. While the first one satisfies at least weakly the constraint of the continuity equation, the latter violates this constraint. Then, we extended the self-consistent approach introducing a new approximation based on the method of equations of motion which satisfies the continuity equation. This approximation is developed in the space of Bogoliubov quasi-particles. The merit of the present method is to reconcile the existence of a gapless spectrum with the absence of divergencies in the vanishing symmetry-breaking limit. At the present, while the extension to systems with many degrees of freedom seems to be straightforward, the validity of PD in higher order truncation schemes is under investigation.

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APPENDIX

In this appendix we show that the continuity equation is satisfied within the approximation performed in this paper. The two independent conditions to be fulfilled are

$$\frac{\sinh 2\theta}{2\nu}e^{-\theta}(\phi_{32} + \phi_{42}) + \phi_{12} + \phi_{22} = -\frac{\lambda}{\nu}e^{-2\theta},\tag{A-1}$$

$$\frac{\sinh 2\theta}{2\nu}e^{-\theta}(\phi_{33} + \phi_{43}) + \phi_{13} + \phi_{23} = 0. \tag{A-2}$$

By writing explicitly the coefficients

$$\frac{\sinh 2\theta}{2\nu}e^{-\theta}\left[2g\nu e^{\theta}\left(2\cosh 2\theta + \sinh 2\theta\right) - 6g\nu e^{\theta}\sinh 2\theta\right] + E_0 = \frac{\lambda}{\nu}e^{-2\theta},\tag{A-3}$$

$$\frac{\sinh 2\theta}{2\nu} e^{-\theta} \left\{ 2 \left[E_0 + g \left(\cosh^2 2\theta + \frac{1}{2} \sinh^2 2\theta \right) \right] - 3g \sinh^2 2\theta \right\}
+ g\nu e^{\theta} \left(2 \cosh 2\theta + \sinh 2\theta \right) - 3g\nu e^{\theta} \sinh 2\theta = 0.$$
(A-4)

The first one reduces simply to

$$2g\sinh 2\theta e^{-2\theta} + E_0 = \frac{\lambda}{\nu} e^{-2\theta},\tag{A-5}$$

which gives exactly the value of E_0 written in Eq. (30) . The second one reads

$$\sinh 2\theta (E_0 + g) + 2g\nu^2 = 0. \tag{A-6}$$

To show that this equality holds we use the condition $\Lambda = 0$ putting it in $E_1 = 0$, which lead to

$$2g\nu^2 + g\sinh 2\theta e^{-4\theta} + \frac{\lambda}{\nu}\sinh 2\theta e^{-2\theta} = 0. \tag{A-7}$$

Due to this condition, Eq. (A-6) becomes

$$\sinh 2\theta \left(\frac{\lambda}{\nu}e^{-2\theta} - 2g\sinh 2\theta e^{-2\theta} + g\right) - \frac{\lambda}{\nu}\sinh 2\theta e^{-2\theta} - g\sinh 2\theta e^{-4\theta} = 0. \tag{A-8}$$

Now, it is simple to show that the left hand side vanishes.

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